

wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 08:59 pm GMT

PDB ID : 6TXZ

Title : FAB PART OF M6903 IN COMPLEX WITH HUMAN TIM3

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Deposited on : 2020-01-15

Resolution : 3.06 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \end{array}$

EDS: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

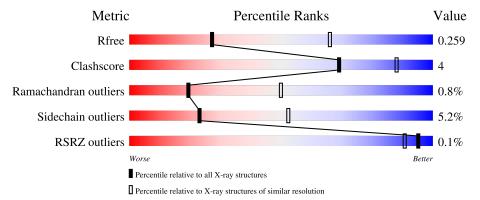
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	A	110	85%	14%	•
1	В	110	92%	7%	•
1	С	110	88%	10%	
1	D	110	92%	6%	••
2	Н	229	82%	13% •	-



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Mol	Chain	Length	Quality of chain	
2	Ι	229	81% 129	6%· 6%
2	J	229	74% 15%	• 8%
2	K	229	79% 13%	• 7%
3	L	214	80% 16	% ••
3	M	214	82%	.5% •
3	N	214	86%	11%
3	О	214	90%	8% •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16053 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Hepatitis A virus cellular receptor 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	109	Total	С	N	О	S	11	0	0
1	A	109	863	550	145	161	7	11	0	U
1	В	109	Total	С	N	О	S	12	0	0
1	В		863	550	145	161	7			U
1	С	109	Total	С	N	О	S	19	0	0
1		109	863	550	145	161	7	13	U	U
1	1 D	D 109	Total	С	N	О	S	10	0	0
1			863	550	145	161	7			U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
A	21	MET	-	initiating methionine	UNP Q8TDQ0
В	21	MET	-	initiating methionine	UNP Q8TDQ0
С	21	MET	-	initiating methionine	UNP Q8TDQ0
D	21	MET	-	initiating methionine	UNP Q8TDQ0

• Molecule 2 is a protein called Fab H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
2	Н	219	Total	С	N	О	S	25	0	0	
2	11	219	1624	1027	270	321	6	20	U		
2	Ţ	216	Total	С	N	О	S	34	24	0	0
2	1	210	1602	1014	266	315	7		U		
2	J	210	Total	С	N	О	S	27	0	0	
2	J	210	1570	998	260	306	6	21	U	U	
2	2 K 213	212	Total	С	N	О	S	21	0	0	
		213	1588	1007	263	311	7	31	U	U	

• Molecule 3 is a protein called Fab L.



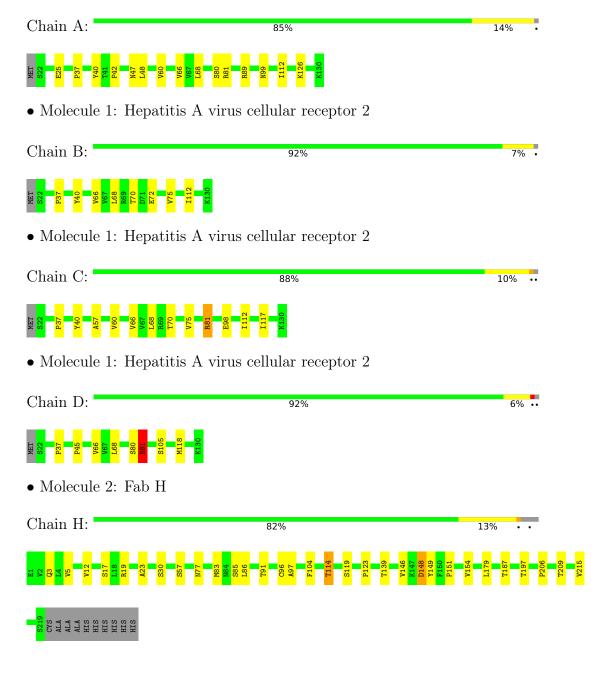
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Т	209	Total	С	N	О	S	21	0	0
3	П	209	1547	967	256	319	5	21	0	U
3	M	210	Total	С	N	О	S	18	0	0
3	1V1		1553	970	257	321	5			
3	N	210	Total	С	N	О	S	49	0	0
3	1	IN 210	1555	971	258	321	5	49	0	U
3	0	911	Total	С	N	О	S	27	0	0
3	3 0	211	1562	975	259	323	5		0	U



3 Residue-property plots (i)

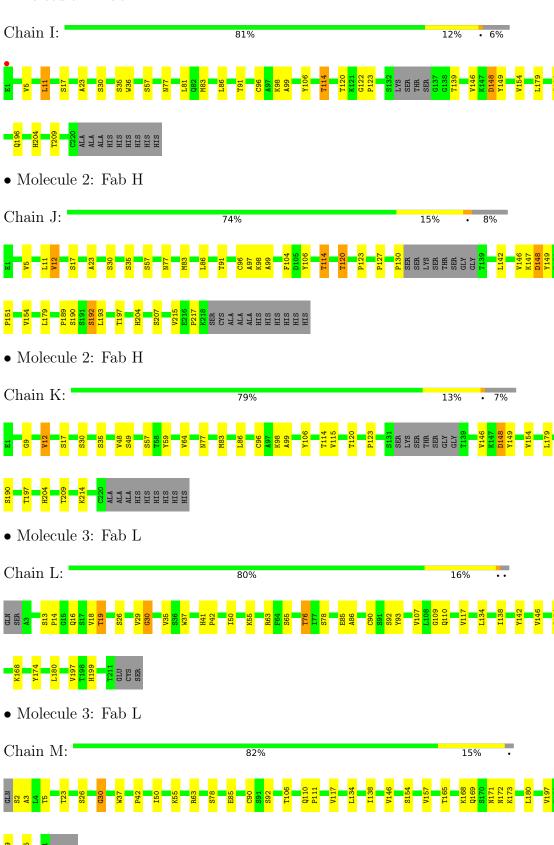
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Hepatitis A virus cellular receptor 2



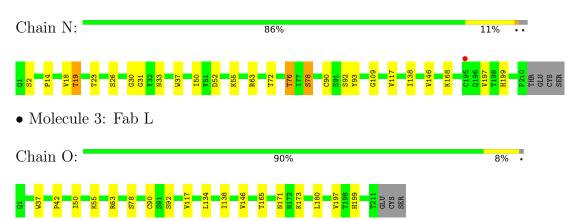








• Molecule 3: Fab L





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	119.35Å 270.12Å 197.89Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 - 3.06	Depositor
Resolution (A)	49.22 - 3.06	EDS
% Data completeness	99.1 (48.60-3.06)	Depositor
(in resolution range)	99.1 (49.22-3.06)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.90 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
D D.	0.197 , 0.253	Depositor
R, R_{free}	0.205 , 0.259	DCC
R_{free} test set	523 reflections $(0.87%)$	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29, 45.2	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16053	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.53	0/884	0.74	0/1202	
1	В	0.50	0/884	0.72	0/1202	
1	С	0.52	0/884	0.74	0/1202	
1	D	0.50	0/884	0.72	0/1202	
2	Н	0.50	0/1664	0.75	0/2266	
2	I	0.43	0/1641	0.69	0/2234	
2	J	0.46	0/1609	0.70	0/2192	
2	K	0.46	0/1627	0.72	0/2216	
3	L	0.50	0/1585	0.73	0/2163	
3	M	0.46	0/1591	0.69	0/2171	
3	N	0.44	0/1593	0.66	0/2173	
3	О	0.49	0/1600	0.68	0/2183	
All	All	0.48	0/16446	0.71	0/22406	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	863	0	832	7	0
1	В	863	0	832	3	0
1	С	863	0	832	7	0
1	D	863	0	832	4	0



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-	110116	DICULUUS	Duuc
	J	1	1

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Н	1624	0	1587	10	0
2	I	1602	0	1561	13	0
2	J	1570	0	1535	22	0
2	K	1588	0	1550	13	0
3	L	1547	0	1496	16	0
3	M	1553	0	1501	12	0
3	N	1555	0	1505	9	0
3	O	1562	0	1512	6	0
All	All	16053	0	15575	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 113 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:138:ILE:HG12	3:M:197:VAL:HG11	1.71	0.72
3:L:138:ILE:HG12	3:L:197:VAL:HG11	1.72	0.71
3:N:138:ILE:HG12	3:N:197:VAL:HG11	1.73	0.68
3:O:138:ILE:HG12	3:O:197:VAL:HG11	1.76	0.66
2:J:127:PRO:HB3	2:J:215:VAL:HG12	1.77	0.64

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	$107/110\ (97\%)$	96 (90%)	9 (8%)	2 (2%)	8 29
1	В	107/110~(97%)	94 (88%)	13 (12%)	0	100 100
1	С	107/110~(97%)	95 (89%)	11 (10%)	1 (1%)	17 47



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	D	107/110 (97%)	96 (90%)	10 (9%)	1 (1%)	17	47
2	Н	217/229 (95%)	209 (96%)	7 (3%)	1 (0%)	29	60
2	I	212/229 (93%)	203 (96%)	8 (4%)	1 (0%)	29	60
2	J	206/229 (90%)	199 (97%)	6 (3%)	1 (0%)	29	60
2	K	209/229 (91%)	198 (95%)	9 (4%)	2 (1%)	15	45
3	L	207/214 (97%)	196 (95%)	9 (4%)	2 (1%)	15	45
3	M	208/214 (97%)	197 (95%)	8 (4%)	3 (1%)	11	36
3	N	208/214 (97%)	199 (96%)	7 (3%)	2 (1%)	15	45
3	О	209/214 (98%)	196 (94%)	12 (6%)	1 (0%)	29	60
All	All	2104/2212 (95%)	1978 (94%)	109 (5%)	17 (1%)	19	50

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	42	PRO
3	M	3	ALA
3	M	42	PRO
3	O	42	PRO
2	Н	148	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	A	94/95~(99%)	91 (97%)	3 (3%)	39	68
1	В	94/95 (99%)	91 (97%)	3 (3%)	39	68
1	С	94/95~(99%)	92 (98%)	2 (2%)	53	77
1	D	94/95 (99%)	90 (96%)	4 (4%)	29	59
2	Н	181/188 (96%)	168 (93%)	13 (7%)	14	40
2	I	178/188 (95%)	167 (94%)	11 (6%)	18	46
2	J	174/188 (93%)	162 (93%)	12 (7%)	15	42



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	K	177/188 (94%)	168 (95%)	9 (5%)	24	53
3	L	175/180 (97%)	166 (95%)	9 (5%)	24	53
3	M	176/180 (98%)	166 (94%)	10 (6%)	20	49
3	N	176/180 (98%)	164 (93%)	12 (7%)	16	42
3	О	177/180 (98%)	172 (97%)	5 (3%)	43	71
All	All	1790/1852 (97%)	1697 (95%)	93 (5%)	23	52

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	18	VAL
3	M	92	SER
3	L	50	ILE
3	L	154	SER
3	M	169	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	77	ASN
3	О	186	GLN
2	K	203	ASN
3	N	110	GLN
2	K	196	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	$\# \mathrm{RSRZ} {>} 2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	109/110 (99%)	-0.42	0 100 100	50, 61, 82, 96	6 (5%)
1	В	109/110 (99%)	-0.40	0 100 100	59, 80, 104, 117	6 (5%)
1	С	109/110 (99%)	-0.46	0 100 100	55, 73, 95, 98	5 (4%)
1	D	109/110 (99%)	-0.47	0 100 100	52, 69, 86, 105	3 (2%)
2	Н	219/229 (95%)	-0.43	0 100 100	46, 61, 85, 115	12 (5%)
2	I	216/229 (94%)	-0.21	1 (0%) 91 79	64, 98, 120, 140	16 (7%)
2	J	210/229 (91%)	-0.36	0 100 100	53, 76, 103, 122	12 (5%)
2	K	213/229 (93%)	-0.34	0 100 100	58, 86, 112, 140	14 (6%)
3	L	209/214 (97%)	-0.41	0 100 100	50, 74, 95, 113	10 (4%)
3	M	210/214 (98%)	-0.45	0 100 100	56, 77, 101, 131	11 (5%)
3	N	210/214 (98%)	-0.24	1 (0%) 91 79	60, 96, 141, 157	20 (9%)
3	О	211/214 (98%)	-0.42	0 100 100	51, 70, 96, 121	10 (4%)
All	All	2134/2212 (96%)	-0.37	2 (0%) 95 91	46, 77, 115, 157	125 (5%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1	GLU	2.0
3	N	195	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

